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NEAR-FIELD THERMAL COUPLING OF A NANOSCALE INTERFACE AND QED KAPITZA CONDUCTANCE OF NANO-CARBON THERMAL INTERCONNECT MATERIALS

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LEHIGH UNIVERSITY

10/26/2015
Final Report

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13. SUPPLEMENTARY NOTES

14. ABSTRACT

Theory of near-field thermal coupling between a nanocarbon material and various substrates was derived. Models were developed to cover a range of nanocarbon dimensions (1D, 0D and 2D), from nanotube films to forests and to graphene layers. A broad range of semiconductor, insulator and metal substrate materials was numerically studied. Materials parameters for optimization of QED Kapitza conductance were determined, including: optimal distance which in turn depends on the frequency of the substrate surface polariton mode and the Fermi velocity or plasmon phase velocity in nanocarbons; optimal width of the thermal interconnect film; large surface polarization of the substrate materials; plasmon frequency of metal substrates; doping level for nanocarbon materials. Analytical models were developed to support the simulations and explain background physics of the process, including non-equilibrium statistical models for strong coupling regime, beyond perturbative solutions. New fundamental effects were uncovered: topological localization of surface polaritons at the nanocarbon wires of lower dimension; development of non-equilibrium (non-thermal) distribution functions of non-perturbatively coupled surface 2D modes. /see Executive summary for the last part of abstract./

15. SUBJECT TERMS

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FINAL PERFORMANCE REPORT

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Contract/Grant Title: Near-field thermal coupling of a nanoscale interface and QED Kapitza conductance of nanocarbon thermal interconnect materials

Contract/Grant #: FA9550-11-1-0185

Reporting Period: 7/15/2011 to 7/14/2014 (with NCE to 7/14/2015)

Abstract:

Theory of near-field thermal coupling between a nanocarbon material and various substrates was derived. Models were developed to cover a range of nanocarbon dimensions (1D, 0D and 2D), from nanotube films to forests and to graphene layers. A broad range of semiconductor, insulator and metal substrate materials was numerically studied. Materials parameters for optimization of QED Kapitza conductance were determined, including: optimal distance which in turn depends on the frequency of the substrate surface polariton mode and the Fermi velocity or plasmon phase velocity in nanocarbons; optimal width of the thermal interconnect film; large surface polarization of the substrate materials; plasmon frequency of metal substrates; doping level for nanocarbon materials. Analytical models were developed to support the simulations and explain background physics of the process, including non-equilibrium statistical models for strong coupling regime, beyond perturbative solutions. New fundamental effects were uncovered: topological localization of surface polaritons at the nanocarbon wires of lower dimension; development of non-equilibrium (non-thermal) distribution functions of non-perturbatively coupled surface 2D modes. Several semi-empirical models were developed or adapted, allowing in the future derivation of compact models for nanocarbon thermal interconnects. Design of thermal coupled devices was performed and initial work on a prototype fabrication was done.

(200 words)

Executive Summary

Cumulative list of people included in the project work (both paid and not paid)

at Lehigh University

- Slava (Vyacheslav) V. Rotkin (PI)
- Andrei M. Nemilentsau (PDA)
- Tetyana Ignatova (GRA)
- Dan You (GRA)
- Negar Moghimi (GRA)
- Nicholas Strandwitz (Prof.)
- Svetlana Tatic-Lucic (Prof.)

at UIUC

- Eric Seabron, Scott Maclaren, Xu Xie (collaborators)

at Ioffe Institute, St.Petersburg

Alexey G. Petrov (collaborator)

at Harvard University (formerly UIUC)

William L. Wilson (collaborator)

at SKKU

Yonghee Lee, Chiongwu Lim (potential collaborators)

at NWU (formerly UIUC)

John A. Rogers (potential collaborator)

Research Summary

During FY1 (2011-2012):

The equilibrium near-field thermal conductance (NFTC) was theoretically studied for carbon nanotube-silica interface[1,2,3,4].

NFTC of the vertical forest of free-standing metallic nanotubes (m-NT) was studied in detail[1].

Materials parameters of both the m-NT and the polar substrate control the magnitude. Kapitza conductance with the magnitude up to 50 MW/K.m can be achieved for a properly designed interface.

A power-law decay of the QED Kapitza conductance vs. the air/vacuum gap has been derived, which allows one to predict such a thermal interconnect material (TIM) to me more robust against delamination or cracking.

Code was written for studying NFTC. The code uses the statistical electrodynamics approach for calculating the partial Kapitza conductance as detailed in Refs.[1,2].

A new phenomenon of plasmon localization in vicinity of the m-NT was observed in numerical simulation.

Nanocarbon TIM performance was assessed for selected dielectric as well as metallic substrates: QED Kapitza conductance was optimized by varying the optical matching conditions of the materials making an interface.

Complementary analytical theory for QED Kapitza conductance was derived for the same interface morphology (m-NT forest) as in the numerical study, as well as for two other morphologies of interest: m-NT film and graphene film[3].

During FY2 (2012-2013):

The study of the fundamentals of the equilibrium NFTC was continued. Obtained results include the following:

A universal model of NFTC was derived for the interface between a nanocarbon TIM of variable dimensionality d=0,1,2 and a polar insulator[5]. This choice of the interface embraces the nanocarbon thermal interconnects made of vertical NT forests, horizontal NT arrays and graphene films.

Electronic and plasmonic mechanisms of NFTC were compared for a representative case of a NT on quartz[6].

Numerical models developed during the first stage[1,2] were extended to cover thermal interfaces between NT forest and metal substrate (for the first time) and non-metal substrates (for a larger class of materials)[7]. The studies[5,8,9] allowed to explain the magnitude of QED Kapitza conductance and its dependence on the materials parameters of the thermal interface, and predict/design the interface which will show the maximal performance.

The characteristic length scale was derived, which determines the range for the QED heat transport mechanism: $L=\omega/v_F \sim 4\text{-}10$ nm. The length scale is influenced by the frequency of the evanescent modes of the substrate, ω, and the density of states of nanocarbon TIM, proportional to the Fermi velocity in nanocarbon materials, v_F. This simple prediction of the analytical theory matches well the numerical model for metal substrates with high values of ω. For the non-metal substrates, the thermal factor was shown to become important, favoring low-ω materials[7].

See Appendix for additional publications, invited talks and seminars.

<u>During FY3 (2013-2014)</u>:

The project has reached the final stage. Results obtained in the project so far has been highlighted in a review article on nanocarbons[10] (along with the cover image for the *Interface* magazine).

The results were intensively disseminated to 6 research groups (RWTH, TMU, JMUW, PUM, UIUC, SKKU), seeking for collaborations for continuing with experimental efforts. Two groups (RWTH, SKKU) expressed interest to fabricate/synthesize samples for experimental verification of the effect. One group (UIUC, Dr. Rogers) expressed interest in receiving theoretical support on related issue of NTFC effect in solar cell devices. Several briefings by PI were conducted in all three groups. The MOI was developed with RWTH/University of Aachen (Dr. Stampfer) and with Center for Integrated Nanostructure Physics, SKKU, Korea (Dr. Y. Lee, Dr. C. Lim).

The study of the plasmonic component of the near-field heat transport was continued beyond the equilibrium approximations, used before. The models were developed for non-equilibrium distribution functions for strongly coupled surface plasmons, contributing to the thermal exchange.

The thermal transfer as a function of frequency (Fourier transform) was found to maximize at the intercepts of dispersion curves of the surface polariton modes of the substrate and the plasmon-polaritons of the nanocarbon material.

For solving the problem of non-equilibrium heat exchange non-Hermitian Green's function method was applied.

Transmission Line Model[11] and Composite Plasmon model were developed to derive compact models for speeding up the numerical simulation of the NFTC in strongly coupled or large scale systems.

Within an analytical model (Green's function method in Lippmann-Schwinger scattering problem) the surface polariton, surprisingly, was found to be bound even by a single nanotube.

See Appendix for additional publications, invited talks and seminars.

(cover image) Tetyana Ignatova, and Slava V. Rotkin, "Discovering Properties of Nanocarbon Materials as a Pivot for Device Applications", cover for Interface, the Electrochemical Society,

v. 22 (3), (2013); Monica Shell, designer; Johanna S. Brams, project manager: IMRC, Lehigh University.

During NCE period (2014-2015):

Non-perturbative solution has been obtained for strongly coupled plasmon modes between 2D and 1D structures[12]. The model explained the role of edge states in finite size NT forests in forming extra branches in differential thermal conductance, observed earlier in numerical simulation[1], and supported modeling of polariton binding on the single NT.

Non-Hermitian Green's function theory has been derived and applied to graphene on SiC[13,14].

Transmission Line model were further studied to apply the theory in the future to near-field thermal measurements via scanning probes[15,16].

The MEMS-like device geometry has been designed, calculated and masks were laid out for experimental verification of the theory predictions. Initial experiments were done to prove the fabrication concept for making the devices[17].

See Appendix for additional publications, invited talks and seminars.

Appendix

Conference/Seminar presentations 2011-2013:

(INVITED)

Alexey G. Petrov, Slava V. Rotkin, “QED Kapitza Conductance of Graphene”, The 221st Meeting of the Electrochemical Society. Seattle, Washington (May 6 - 11, 2012).

Slava V. Rotkin, Alexey G. Petrov, “QED Kapitza Conductance of Nanocarbon Materials: From Fundamental Physics to Applications”, the 2012 Energy, Materials and Nanotechnology Meeting, Villa Conference on Interaction Among Nanostructures. Orlando, FL, April 16-20, 2012.

Slava V. Rotkin, “Near-Field Heat Transport in Nanocarbons: Go Quantum – Go Cool”, seminar at National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL (Apr 13, 2012).

(CONTRIBUTED)

Slava V. Rotkin, Alexey G. Petrov, “An Essential Mechanism of Heat Dissipation in Nanocarbon Electronics”, 2013 APS March Meeting, March 18–22, 2013; Baltimore, Maryland.

Andrei M. Nemilentsau, and Slava V. Rotkin, “Plasmon Heat Transport Between Vertical Carbon Nanotube Forest and Different Substrates”, 2013 APS March Meeting, March 18–22, 2013; Baltimore, Maryland.

Slava V. Rotkin, Alexey G. Petrov, Andrei M. Nemilentsau, "QED Interfacial Heat Conductance in Nanocarbon Thermal Interconnects", 2012 Workshop on Innovative Nanoscale Devices and Systems, December 2-7, 2012. Hapuna Beach Prince Hotel, Kohala Coast, Hawaii, USA.

Andrei M. Nemilentsau, Slava V. Rotkin, “Nanoscale radiative heat transfer between a dielectric substrate and an SWNT”, The 221st Meeting of the Electrochemical Society. Seattle, Washington (May 6 - 11, 2012).

(POSTER)

Dan You, and Slava V. Rotkin, “Plasmonic heat transfer between graphene and dielectric substrate”, 2013 APS March Meeting, March 18–22, 2013; Baltimore, Maryland. [Bulletin of the APS March Meeting, 58 (1), V1.00016 (2013).]

Conference/Seminar presentations in 2013-2014:

(INVITED)

Slava V. Rotkin, “Physics of Nanocarbon: Nobel Prize, Kavli Prize,... What's Next?”, REU special lecture, Lehigh University, 28 June 2013.

Alexey G. Petrov, Andrei. M. Nemilentsau, and Slava V. Rotkin, “Plasmonic vs. electronic mechanism of the QED Kapitza Conductance for nanotube materials”, the 223rd Meeting of the Electrochemical Society; Toronto, Ontario, Canada (May 12-17, 2013).

Slava V. Rotkin, “Heat Tunneling in Nanocarbons: Near-field Cross-plane Thermal Transport”, MRL seminar, 10 December 2013, UIUC, Urbana, IL.

Slava V. Rotkin, “Electronic properties and near field optics of SWNT complexes”, Seminar at Technical University of Munich, 8 November 2013, Munich, Germany.

Slava V. Rotkin, “Pure surface or Tainted interface: On scattering in the single layer graphene”, Condensed Matter Seminar, RWTH/Aachen University, 24 September 2013, Aachen, Germany.

Slava V. Rotkin, “QED Heat Tunneling Across Nanocarbon Interface”, CINAP/IBS seminar, 9 January 2014, SKKU, Suwon, Korea.

Slava V. Rotkin, “Interfacial heat transport in graphene and across NT forests: Theory of QED Kapitza conductance in nanocarbons”, The 1st Muju International Winter School Series, Muju Deogyusan Resort, Republic of Korea (9-15 Feb 2014).

Slava V. Rotkin, “Physics of Nanocarbon: Nobel Prize, Kavli Prize,... What's Next?”, REU special lecture, Lehigh University, 18 July 2014.

Conference/Seminar presentations in 2015:

(INVITED)

Slava V. Rotkin, “Nanophotonics with Nanocarbon Materials: From Bio-sensing to Remote Heat Removal” (keynote), Advances in Functional Materials, Stony Brook University, USA (Jun 29 - Jul 3, 2015).

Slava V. Rotkin, “Physics of QED Interfacial Heat Conductance in Nanocarbons”, Beckman Institute 25th anniversary Symposium, October 9-10, 2014. Beckman Institute, UIUC, Urbana, IL.

(CONTRIBUTED)

Dan You and Slava V. Rotkin, “Non-equilibrium thermodynamics approach for QED heat conductance between graphene and SiC substrate”, the 227th Meeting of the Electrochemical Society. Chicago, IL (2015, May 24-28).

Slava V. Rotkin, “Analytical quantitative theory of RF-SPM for nanocarbon electronics”, 2015 APS March Meeting, March 2-6, 2015. San Antonio, Texas. [Bulletin of the APS March Meeting, 60 (2), F21.00005 (2015).]

Publications that stem from the grant:

[1] Andrei M. Nemilentsau, and Slava V. Rotkin, “Vertical Single-Wall Carbon Nanotube Forests as Plasmonic Heat Pipes”, ACS Nano 6 (5), 4298-4304 (2012).DOI: 10.1021/nn300848b

[2] Tetyana Ignatova, Andrei M. Nemilentsau, and Slava V. Rotkin, “Near-field optics of SWNTs and FRET in their nanoscale complexes”, in Handbook on Carbon Nano Materials, ed. F DiSouza, K Kadish. World Scientific Publishing, Inc. (2012), Chapter 18.

[3] Slava V. Rotkin, Alexey G. Petrov, “QED Kapitza Conductance of Nano-Carbon Materials: From Fundamental Physics to Applications”, in Proceedings of the Villa Conference on Interaction Among Nanostructures. Kimberly A. Sablon and Zhiming M. Wang, (Villa, FL, April 16-20, 2012).

[4] Alexey G. Petrov, Slava V. Rotkin, “QED Kapitza Conductance of Graphene”, in Proceedings of The 221st Meeting of the Electrochemical Society. (Seattle, WA, May 6-11, 2012).

[5] Slava V. Rotkin, Alexey G. Petrov, Andrei M. Nemilentsau, "QED Interfacial Heat Conductance in Nanocarbon Thermal Interconnects", in Proceedings of Workshop on Innovative Nanoscale Devices and Systems, Eds. Koji Ishibashi, Stephen M. Goodnick, Siegfried Selberherr, Akira Fujiwara (12/2-7/12, Kohala Coast, Hawaii, USA). ISBN 978-3-901578-25-0

[6] Alexey G. Petrov, Andrei. M. Nemilentsau, and Slava V. Rotkin, "Plasmonic vs. electronic mechanism of the QED Kapitza Conductance for nanotube materials", in Proceedings of the 223rd Meeting of the Electrochemical Society; (Toronto, Ontario, Canada; May 12-17, 2013).

[7] Andrei M. Nemilentsau, and Slava V. Rotkin, "Optimization of nanotube thermal interconnects for near-field radiative heat transport", Applied Physics Letters 101, 063115 (2012). DOI:10.1063/1.4745202

[8] Slava V. Rotkin, Alexey G. Petrov, "An Essential Mechanism of Heat Dissipation in Nanocarbon Electronics", Bulletin of the APS March Meeting, 58 (1), G7.00004 (2013).

[9] Andrei M. Nemilentsau, and Slava V. Rotkin, "Plasmon Heat Transport Between Vertical Carbon Nanotube Forest and Different Substrates", Bulletin of the APS March Meeting, 58 (1), Z7.00011 (2013).

[10] Tetyana Ignatova, and Slava V. Rotkin, "Discovering Properties of Nanocarbon Materials as a Pivot for Device Applications", Interface of the Electrochemical Society, v. 22, N 3, pp. 49-52 (2013).

[11] Slava V. Rotkin, Eric Seabron, Scott Maclaren, Xu Xie, John A. Rogers, and William L. Wilson, "Transmission Line Model for Microwave Fast Scanning Tool: Theoretical Backgrounds for Nanotube Nano-Characterization", in Proceedings of Workshop on Innovative Nanoscale Devices and Systems, Eds. Viktor Sverdlov, Berry Jonker, Siegfried Selberherr, Koji Ishibashi, Stephen M. Goodnick, (12/1-5/14, Kohala Coast, Hawaii, USA). ISBN 978-3-901578-28-1.

[12] Alexey G. Petrov, Slava V. Rotkin, "Efficiency of nanotube materials as plasmonic thermal interconnects: Theory of bound polariton modes", in preparation.

[13] Dan You and Slava V. Rotkin, "Non-equilibrium thermodynamics approach for QED heat conductance between graphene and SiC substrate", in Proceedings of the 227th Meeting of the Electrochemical Society; (Chicago, IL, 2015 May 24 - 28), 2015.

[14] Dan You and Slava V. Rotkin, "Non-equilibrium distribution of plasmon-polaritonic modes beyond perturbation theory: QED heat conductance between graphene and SiC substrate", in preparation.

[15] Eric Seabron, Scott MacLaren, Xu Xie, Slava V. Rotkin, John A. Rogers, and William L. Wilson, "Scan-probe microwave reflectivity of single walled carbon nanotubes: Nanoscale permittivity imaging in the quantum regime", ACS Nano, submitted (2015).

[16] Slava V. Rotkin, "Thermal contribution of plasmonic modes in QED Kapitsa conductance: Analytical results with Transmission Line model", in preparation.

[17] Negar Moghimi, Nicholas Strandwitz, Svetlana Tatic-Lucic, and Slava V. Rotkin "Demonstration of lift-off micro-patterning for atomic layer deposited titanium oxide", in preparation.

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Grant/Contract Number
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Principal Investigator Name
The full name of the principal investigator on the grant or contract.

Vyacheslav V. Rotkin

Program Manager
The AFOSR Program Manager currently assigned to the award

Dr. Ali Sayir, AFOSR/RTD

Reporting Period Start Date

07/15/2011

Reporting Period End Date

07/14/2015

Abstract

Theory of near-field thermal coupling between a nanocarbon material and various substrates was derived. Models were developed to cover a range of nanocarbon dimensions (1D, 0D and 2D), from nanotube films to forests and to graphene layers. A broad range of semiconductor, insulator and metal substrate materials was numerically studied. Materials parameters for optimization of QED Kapitza conductance were determined, including: optimal distance which in turn depends on the frequency of the substrate surface polariton mode and the Fermi velocity or plasmon phase velocity in nanocarbons; optimal width of the thermal interconnect film; large surface polarization of the substrate materials; plasmon frequency of metal substrates; doping level for nanocarbon materials. Analytical models were developed to support the simulations and explain background physics of the process, including non-equilibrium statistical models for strong coupling regime, beyond perturbative solutions. New fundamental effects were uncovered: topological localization of surface polaritons at the nanocarbon wires of lower dimension; development of non-equilibrium (non-thermal) distribution functions of non-perturbatively coupled surface 2D modes. Several semi-empirical models were developed or adapted, allowing in the future derivation of compact models for nanocarbon thermal interconnects. Design of thermal coupled devices was performed and initial work on a prototype fabrication was done.

Main contributors to the project were: Slava (Vyacheslav) V. Rotkin (PI), Andrei M. Nemilentsau (PDA), Tetyana Ignatova (GRA), Dan You (GRA), Negar Moghimi (GRA), Nicholas Strandwitz (Prof.), Svetlana Tatic-Lucic (Prof.) -- all at Lehigh University; and Dr. Alexey G. Petrov (collaborator at Ioffe Institute, St.Petersburg).

The list of publications that stem from this grant includes 17 items, listed in appendix to Executive Summary, as well as additional list of presentations made during the term of the project and acknowledging AFOSR support.

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Archival Publications (published) during reporting period:

Andrei M. Nemilentsau, and Slava V. Rotkin, “Vertical Single-Wall Carbon Nanotube Forests as Plasmonic Heat Pipes”, ACS Nano 6 (5), 4298-4304 (2012).DOI: 10.1021/nn300848b

Tetyana Ignatova, Andrei M. Nemilentsau, and Slava V. Rotkin, “Near-field optics of SWNTs and FRET in their nanoscale complexes”, in Handbook on Carbon Nano Materials, ed. F DiSouza, K Kadish. World Scientific Publishing, Inc. (2012), Chapter 18.

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Andrei M. Nemilentsau, and Slava V. Rotkin, “Plasmon Heat Transport Between Vertical Carbon Nanotube Forest and Different Substrates”, Bulletin of the APS March Meeting, 58 (1), Z7.00011 (2013).

Tetyana Ignatova, and Slava V. Rotkin, “Discovering Properties of Nanocarbon Materials as a Pivot for Device Applications”, Interface of the Electrochemical Society, v. 22, N 3, pp. 49-52 (2013).

Slava V. Rotkin, Eric Seabron, Scott Maclaren, Xu Xie, John A. Rogers, and William L. Wilson, "Transmission Line Model for Microwave Fast Scanning Tool: Theoretical Backgrounds for Nanotube Nano-Characterization", in Proceedings of Workshop on Innovative Nanoscale Devices and Systems, Eds. Viktor Sverdlov, Berry Jonker, Siegfried Selberherr, Koji Ishibashi, Stephen M. Goodnick, (12/1-5/14, Kohala Coast, Hawaii, USA). ISBN 978-3-901578-28-1.

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Changes in research objectives (if any):

Change in AFOSR Program Manager, if any:

(originally) Dr. Kumar Jata
(formerly) Dr. Joan Fuller
(currently) Dr. Ali Sayir

Extensions granted or milestones slipped, if any:

NCE granted in 2014

AFOSR LRIR Number

LRIR Title

Reporting Period

Laboratory Task Manager

Program Officer

Research Objectives

Technical Summary

Funding Summary by Cost Category (by FY, $K)

	Starting FY	FY+1	FY+2
Salary			
Equipment/Facilities			
Supplies			
Total			

Report Document

Report Document - Text Analysis

Report Document - Text Analysis

Appendix Documents

2. Thank You

E-mail user

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